

Accidental Degeneracy and Berry Phase of Resonant States

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Abstract

We study the complex geometric phase acquired by the resonant states of an open quantum system which evolves irreversibly in a slowly time dependent environment. In analogy with the case of bound states, the Berry phase factors of resonant states are holonomy group elements of a complex line bundle with structure group \mathbf{C}^* . In sharp contrast with bound states, accidental degeneracies of resonances produce a continuous closed line of singularities formally equivalent to a continuous distribution of “magnetic” charge on a “diabolical” circle, in consequence, we find different classes of topologically inequivalent non-trivial closed paths in parameter space.

1 Introduction.

For many years now, it has been appreciated that there are distinct advantages in describing quantum resonances and the quantum phenomena associated to the production, evolution and decay of resonances in terms of resonant or Gamow states, since many physical effects are then readily expressed and evaluated[1]. In this work, we will give closed analytical expressions for the complex Berry phase of an open quantum system in a resonant state of a Hermitian Hamiltonian with non-self-adjoint boundary conditions, and we will discuss some of its properties.

During the last fourteen years the geometric phase factors arising in the adiabatic evolution of quantum systems[2] have been the subject of many investigations[3, 4]. The early literature was mostly concerned with the geometric phase factors of closed systems driven by Hermitian Hamiltonians[4]. More recently there has been a substantial interest in the complex geometric phase acquired by the eigenstates of open quantum systems. This problem arises naturally in connection with various experiments which, by their very essence, require the observation of the geometric phase in metastable states. The Berry phase in the optical supermode propagation in a free laser, which is a classical system described by a Schrödinger-like equation with a non-Hermitian Hamiltonian, was studied by Dattoli et al.[5]. The measurement of the

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geometric phase in atomic systems with two energy levels, one of which at least is metastable, was also described in terms of a non-Hermitian Hamiltonian by Miniatura et al.[6]. The validity of the adiabatic approximation for dissipative, two level systems driven by non-Hermitian Hamiltonians was examined by Nenciu and Rasche[7], and by Kvitsinsky and Putterman[8], who also established that the Berry phase is complex in this case. Sun[9] proposed a higher-order adiabatic approximation for two-level non-Hermitian Hamiltonians, and showed that the holonomy structure associated to the Berry phase factor in this non-Hermitian case is the non-unitary generalization of the holonomy structure of the Hermitian case.

In two previous papers[10, 11], we gave explicit expressions for the geometric phase of true resonant states, defined as complex energy eigenstates of a Hermitian Hamiltonian which satisfy purely outgoing wave boundary conditions at infinity[12], and pointed out some of the mathematically interesting and physically relevant properties resulting from the extended nature of the singularities in parameter space associated with the occurrence of accidental degeneracies of two resonances. In this connection, in another paper we showed that the codimension of the accidental degeneracy of n resonances differ significantly from those of bound states, we also showed that, close to a crossing of two resonant states, the topological structure of the energy hypercomplex surfaces differ significantly from the double conical point singularity typical of bound states[13]. Later, by means of a numerical analysis of the experimental data on the 2^+ doublet of resonances with $T = 0, 1$ in the energy spectrum of ^8Be , we showed, in a realistic example, that a true crossing of resonances mixed by a Hermitian interaction may be brought about by the variation of only two real linearly independent parameters[14]. In this paper we show that the geometric interpretation of the Berry phase factor, first given by B. Simon[15] for the adiabatic evolution of closed quantum systems, may be generalized, in a very natural way, to the case of resonant states of open quantum systems. That is, the adiabatic evolution of resonant states may be interpreted as parallel transport in a complex line bundle defined over the space of parameters with structure group \mathbf{C}^* (the multiplicative group of the non-zero complex numbers). Then, the Berry phase factors of resonant states arise as the holonomy group elements due to a connection in the bundle such that during the adiabatic evolution the resonant state is parallel transported along the fibre. The horizontal spaces are perpendicular to the fibre with respect to a generalized inner product of resonant states defined in a rigged Hilbert space.

2 Resonant States

2.1 Resonant states in a slowly time evolving environment

Let us consider the time evolution of a quantum system in a state which is a superposition of unstable eigenstates moving in some strong external field of force which changes slowly with time. In order to have some concrete example in mind, although a very hypothetical one, we may think of an ^8Be nucleus which

has only unstable energy eigenstates moving in the field of forces of a double magic nucleus, like ^{208}Pb , in a peripheral collision in which the distance between the two nuclei is never smaller than the sum of the nuclear radii. In a semiclassical treatment of the collision, when the centers of the nuclei move along classical trajectories, the parameters in the nucleus-nucleus interaction change with time[16].

The evolution of the system under the influence of the external perturbation is governed by the time dependent Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = H \Psi. \quad (1)$$

The Hamiltonian H is the sum of the time-independent Hamiltonian H_0 describing the evolution of the unperturbed system plus a perturbation term H_1 which is a function of a number N of “external” parameters $\{X_1, X_2, \dots, X_N\}$ which may change with time,

$$H(t) = H_0 + H_1(X_i(t)). \quad (2)$$

The energy eigenfunctions of the unperturbed Hamiltonian are the solutions of the equation,

$$H_0 \varphi_m(\xi_i, \eta_j, r) = \mathcal{E}_m \varphi_m(\xi_i, \eta_j, r), \quad (3)$$

the wave functions $\varphi_m(\xi_i, \eta_j, r)$ satisfy the boundary conditions appropriate to a decaying state.

Assuming that, in the absence of perturbation, the unstable system decays spontaneously in two stable fragments, the unperturbed energy eigenfunctions may be written as cluster model wave functions[17]

$$\varphi_m(\xi_i, \eta_j, r) = \mathcal{A} \left\{ \phi_A(\xi_i) \phi_B(\eta_j) \frac{u_{ml}(r)}{r} \mathcal{Y}_{Jls}^M(\hat{r}) \right\}. \quad (4)$$

where $\phi_A(\xi_i)$ and $\phi_B(\eta_j)$ are the wave functions of the clusters A and B, $u_{ml}(r)$ is the radial part of the wave function of the relative motion of the two clusters, $\mathcal{Y}_{Jls}^M(\hat{r})$ is a spherical harmonic and \mathcal{A} is the antisymmetrizer. In our example, φ_m would be the eigenfunction of a state of ^8Be which decays spontaneously in two ^4He clusters. In this case $u_{ml}(r)$ is a Gamow function.

2.2 A few facts about Gamow functions

Gamow functions are the eigenfunctions of the time independent Schrödinger equation which vanish at the origin, and behave as purely outgoing waves for large values of the relative distance r ,

$$u_{ml}(0) = 0, \quad (5)$$

and

$$\lim_{r \rightarrow \infty} [u_{ml}(r) - O_l(k_m, r)] = 0, \quad (6)$$

where the function $O_l(k_m, r)$ is an outgoing spherical wave of complex wave number k_m and angular momentum l [12].

The boundary condition (6) is not self-adjoint, in consequence, the energy eigenvalues are complex, with $Re\mathcal{E}_m > 0$ and $Im\mathcal{E}_m < 0$. Hence, Gamow functions are a generalization of bound state eigenfunctions in that they belong to complex wave numbers, $k_m = \kappa_m - i\gamma_m$, with $\kappa_m > \gamma_m > 0$, instead of purely imaginary ones. This generalization leads out of the Hilbert space based quantum mechanics. Therefore, the quantum mechanical rules for normalization, orthogonality and completeness in their usual form, do not apply. Nevertheless, bound and resonant states form a bi-orthonormal set with their adjoints, which may be extended by a continuum of suitably chosen scattering states of complex wave number to form a complete set in terms of which any square integrable function may be expanded [12].

The symmetry properties of the Schrödinger equation and the boundary conditions under the operations of complex conjugation and reversal of time suggest a definition for the adjoint $\tilde{u}_{ml}(k_m, r)$ of the Gamow function $u_{ml}(k_m, r)$ [12],

$$\tilde{u}_{ml}(k_m, r) = u_{ml}^*(-k_m^*, r). \quad (7)$$

Now, if the adjoint $\tilde{u}_{ml}(k_m, r)$ is identified with the bra-eigenfunction, the quantum mechanical inner product, or bra-c-ket rule, may be generalized to include Gamow eigenfunctions. With this prescription, matrix elements of operators and inner products are computed in configuration space representation as integrals over the radial variable r . Since the Gamow function $u_{ml}(k_m, r)$ and its adjoint $\tilde{u}_{ml}(k_m, r)$ oscillate between envelopes that grow exponentially with r , the integrals over r must be properly defined. This may be done, either by analytic continuation in the complex k -plane from above [12, 18] or by means of an Abel regulator[19] with a suitable convergence factor and a limiting procedure[20, 21]. Both procedures give the same result[22, 23]. In this paper, we will adopt the second definition.

Then, it may be shown that

$$\lim_{\mu \rightarrow 0} \int_0^\infty e^{-\mu r^2} u_{ml}^*(-k_m^*, r) u_{nl'}(k_n, r) dr = \delta_{mn} \delta_{ll'} \quad (8)$$

i.e, the Gamow eigenfunctions are orthonormalized in a generalized sense. It may also be shown[12, 24] that, for any two square integrable functions, $f(r)$ and $g(r)$, the following relation holds

$$\begin{aligned} \int_0^\infty f^*(r) g(r) dr = \sum_n \{ [\int_0^\infty f^*(r) u_{nl}(k_n, r) dr] \times [\int_0^\infty u_{nl}^*(-k_n^*, r') g(r') dr'] \} + \\ \int_c dk [\int_0^\infty f^*(r) \phi_l(k, r) dr] [\int_0^\infty \phi_l^*(-k^*, r') g(r') dr'] . \end{aligned} \quad (9)$$

In this expression, the functions $u_{nl}(r)$ are bound states or Gamow state eigenfunctions belonging to real negative or complex eigenvalues \mathcal{E}_n , the functions $\phi_l(k, r)$ are scattering partial wave functions of angular momentum l and complex wave number k . The integration contour C , in the wave number plane k , starts from the origin as a straight line with slope -1, it goes down to $Imk = \alpha$ and then, it continues as a straight line parallel to the real axis[12]. Finally, the square brackets around the integrals mean that, when necessary, the integrals are defined by means of a gaussian regulator and a limit as in (8) or by analytical continuation from above as in Mondragón and Hernández[12, 24].

Since $f(r)$ and $g(r)$ are arbitrary functions, we are justified in writing the expansion

$$g(r) = \sum_m u_{ml}(r) \langle u_{ml} | g \rangle + \int_C \phi_l(k, r) \langle \phi_l(k) | g \rangle dk, \quad (10)$$

the index m runs over bound and resonant states.

The expansion coefficients are given by

$$\langle u_{ml} | g \rangle = \lim_{\mu \rightarrow 0} \int_0^\infty e^{-\mu r^2} u^*(-k_m^*, r) g(r) dr, \quad (11)$$

$$\langle \phi_l(k) | g \rangle = \lim_{\mu \rightarrow 0} \int_0^\infty e^{-\mu r^2} \phi_l^*(-k^*, r) g(r) dr. \quad (12)$$

Once the validity of the quantum mechanical inner product has been generalized to apply to bound and resonant eigenfunctions of the relative motion of the two clusters, the generalization of (9) and (10) to expansions of many body wave functions in terms of cluster model bound and resonant eigenfunctions is fairly straightforward[12, 24].

2.3 The mixing matrix

We may, now, go back to our problem, namely the time evolution of the resonant states of a many body system moving in a slowly time-dependent external field of force. Since we are interested in the time evolution of a state Ψ which is a superposition of unstable states, we make an expansion of the wave function Ψ in terms of bound and resonant states of H_0 ,

$$\Psi = \sum_m a_m(t) \varphi_m(\xi_i, \eta_j, r) + \int_C b(k; t) \varphi^{(+)}(k; \xi_i, \eta_j, r) dk. \quad (13)$$

In general, the index m runs over bound and resonant states. In our example, φ_m would be the complex energy eigenfunctions of the ^8Be nucleus which decays spontaneously in two ^4He clusters. The scattering states $\varphi^{(+)}(k, \xi_i, \eta_j, r)$ of complex wave number k and the integration contour C are defined in the previous subsection.

Substitution of (13) in (1) gives the set of coupled equations

$$\frac{da_m(t)}{dt} = -\frac{i}{\hbar}\mathcal{E}_m a_m(t) - \frac{i}{\hbar} \sum_n \langle \varphi_m | H_1(t) | \varphi_n \rangle a_n(t) - \frac{i}{\hbar} \int_c \langle \varphi_m | H_1(t) | \varphi^{(+)}(k) \rangle b(k; t) dk \quad (14)$$

and a similar expression for $db(k, t)/dt$.

We will use the notation $|\varphi_m(\xi_i, \eta_j, r) \rangle$ for the Gamow function, and $\langle \varphi_m(\xi_i, \eta_j, r) |$ for its adjoint. Hence, the matrix element of the perturbation term $H_1(t)$ taken between bound or resonant states of the unperturbed system is given by

$$\langle \varphi_m | H_1(t) | \varphi_n \rangle = \int \cdots \int \langle \varphi_m(\xi_i, \eta_j, r) | H_1(t) | \varphi_n(\xi_i, \eta_j, r) \rangle d^3 \xi_1 \cdots d^3 \xi_{A-1} d^3 \eta_1 \cdots d^3 \eta_{B-1} d^3 r, \quad (15)$$

the integral over the radial variable r is defined as in (8).

When the interactions are time reversal invariant, the dual of the complex Gamow function $u_{ml}(r)$ is the same function[12, 21, 24]. But, when the interactions are not time reversal invariant, the Gamow function and its dual are not the same function.

Therefore, when the forces acting on the system are time reversal invariant, the complex matrix \mathbf{H} , with matrix elements

$$\mathbf{H}_{mn}(t) = \mathcal{E}_m \delta_{mn} + \langle \varphi_m | H_1(t) | \varphi_n \rangle \quad (16)$$

is symmetric but non-Hermitian. When the forces acting on the system are not time reversal invariant, \mathbf{H} is, in general, complex, non-symmetric and non-Hermitian.

The contribution of the non-resonant background integral over the continuum of scattering wave functions to (13) and (14) will not be relevant to the following discussion. Therefore, to ease the notation, we will disregard the contribution of the background of scattering functions. With this truncation,

$$H\Psi = \sum_m |\varphi_m(\xi_i, \eta_j, r) \rangle \left[\sum_n \mathbf{H}_{mn} a_n(t) \right]. \quad (17)$$

Then, the set of coupled equations(14) reduces to

$$\dot{a}_m(t) = -\frac{i}{\hbar} \sum_n \mathbf{H}_{mn} a_n(t), \quad (18)$$

where $\dot{a}_m(t)$ is the time derivative of $a_m(t)$.

3 Geometric Phase of a Resonant State.

The time evolution of the quantum system is governed by the Hamiltonian H , or the matrix \mathbf{H} , which are functions of N real, linearly independent parameters. Therefore, we may consider the matrix \mathbf{H} embedded

in a population of \mathbf{H} matrices smoothly parametrized by N external parameters which take values in some domain D of a manifold or parameter space. Each point in D represents an \mathbf{H} matrix. When the external parameters change with time, the system traces a path C in parameter space. In the following, we will study the behaviour of the system in the time interval $[0, T]$, assuming that at the initial time, $t = 0$, it is in an eigenstate of \mathbf{H} , at $t = T$ the parameters (X_1, X_2, \dots, X_N) have returned to their initial values, and the adiabatic theorem holds. Then, the unstable system traces a closed path C in parameter space while it remains in an eigenstate of $\mathbf{H}(t)$ at all times.

In the absence of symmetry, \mathbf{H} has no repeated eigenvalues at almost all points in the domain D . The set of points in D where \mathbf{H} has one twofold repeated eigenvalue is a subdomain $D' \subset D$. If D has N dimensions, and D' has N' dimensions, then $N = N' + \kappa$, κ is the codimension of the twofold degeneracy. Similar relations hold in the case of an m -fold degeneracy.

It will be assumed that the complex non-Hermitian matrix \mathbf{H} has no repeated eigenvalues at all points on the path C . In consequence, at all points on C , it may be brought to diagonal form by means of a similarity transformation

$$\mathbf{K}^{-1}\mathbf{H}\mathbf{K} = \mathbf{E}, \quad (19)$$

where \mathbf{E} is the diagonal matrix of the complex energy eigenvalues. The columns in the matrix \mathbf{K} are the instantaneous right eigenvectors of \mathbf{H} . In an obvious notation

$$\mathbf{K} = \left(|\phi^{(1)}\rangle, |\phi^{(2)}\rangle, \dots, |\phi^{(s)}\rangle, \dots, |\phi^{(n)}\rangle \right). \quad (20)$$

which satisfy the eigenvalue equation

$$\mathbf{H}(X_l(t)) |\phi^{(s)}(t)\rangle = \mathcal{E}_s(t) |\phi^{(s)}(t)\rangle. \quad (21)$$

The rows in \mathbf{K}^{-1} are the corresponding left eigenvectors of \mathbf{H} , properly normalized,

$$\langle \phi^{(i)} | \phi^{(j)} \rangle = \delta_{ij}. \quad (22)$$

The adiabatic basis, $\{ |\hat{\varphi}_s(\xi_i, \eta_j, r; X_l(t))\rangle \}$, of instantaneous bound and resonant energy eigenstates of the complete Hamiltonian H , is obtained from the set of unperturbed bound and resonant states with the help of the matrix \mathbf{K}

$$|\hat{\varphi}_s(\xi_i, \eta_j, r; X_l(t))\rangle = \sum_m |\varphi_m(\xi_i, \eta_j, r)\rangle \mathbf{K}_{ms}(t) \quad (23)$$

and their adjoints (duals) are given by

$$\langle \hat{\varphi}_s(\xi_i, \eta_j, r; X_l(t)) | = \sum_n (\mathbf{K}^{-1}(t))_{sn} \langle \varphi_n(\xi_i, \eta_j, r) |. \quad (24)$$

It follows that the instantaneous bound and resonant energy eigenstates of $H(t)$ satisfy an orthogonality relation similar to (8), which they inherit from the unperturbed complex energy eigenfunctions

$$\begin{aligned} \langle \hat{\varphi}_s(\xi_i, \eta_j, r; X_l(t)) | \hat{\varphi}_{s'}(\xi_i, \eta_j, r; X_l(t)) \rangle &= \sum_{m,n} (\mathbf{K}^{-1})_{sn} \langle \varphi_n(\xi_i, \eta_j, r) | \varphi_m(\xi_i, \eta_j, r) \rangle \mathbf{K}_{ms'} = \\ &= \sum_{m,n} (\mathbf{K}^{-1})_{sn} \delta_{nm} \mathbf{K}_{ms'} = \delta_{ss'}. \end{aligned} \quad (25)$$

If we multiply both sides of eq.(23) by \mathbf{K}^{-1} , we obtain

$$|\varphi_m(\xi_i, \eta_j, r)\rangle = \sum_s |\hat{\varphi}_s(\xi_i, \eta_j, r; X_l(t))\rangle (\mathbf{K}^{-1})_{sm}. \quad (26)$$

Substitution of this expression in (13), gives the expansion of Ψ in instantaneous energy eigenfunctions of \mathbf{H} ,

$$\Psi = \sum_s |\hat{\varphi}_s(\xi_i, \eta_j, r; X_l(t))\rangle \hat{a}_s(t), \quad (27)$$

where

$$\hat{a}_s(t) = \sum_n (\mathbf{K}^{-1}(t))_{sn} a_n(t). \quad (28)$$

In (27) we have kept only the summation over bound and resonant states and, as in the previous section, we have disregarded the contribution from the integral over the continuum of scattering functions of complex wave number.

Similarly, the expansion of $H\Psi$ becomes

$$H\Psi = \sum_s |\hat{\varphi}_s(\xi_i, \eta_j, r; X_l(t))\rangle \hat{\mathcal{E}}_s(t) \hat{a}_s(t). \quad (29)$$

Substitution of (27) and (29) in the time dependent Schrödinger equation gives the set of coupled equations

$$\frac{d\hat{a}_s(t)}{dt} + \sum_{m=1} \langle \hat{\varphi}_s | \nabla_{\mathfrak{R}} \hat{\varphi}_m \rangle \cdot \frac{d\vec{\mathfrak{R}}}{dt} \hat{a}_m(t) = -i\hat{\mathcal{E}}_s(t) \hat{a}_s(t) \quad (30)$$

where, $|\nabla_{\mathfrak{R}} \hat{\varphi}_m \rangle$ is the gradient of $|\hat{\varphi}_m \rangle$ in parameter space,

$$\frac{d|\hat{\varphi}_m \rangle}{dt} = \sum_{i=1}^N \left(\frac{\partial}{\partial X_i} |\hat{\varphi}_m \rangle \right) \frac{dX_i}{dt} = |\nabla_{\mathfrak{R}} \varphi_m \rangle \cdot \frac{d\vec{\mathfrak{R}}}{dt} \quad (31)$$

It will be assumed that the non-adiabatic transition amplitudes are very small

$$\frac{1}{|\hat{a}_s|} \left| \langle \hat{\varphi}_s | \nabla_{\mathbb{R}} \hat{\varphi}_m \rangle \cdot \frac{d\vec{\mathcal{R}}}{dt} \right| \ll 1, \quad m \neq s. \quad (32)$$

Then, we can make the approximation

$$\frac{1}{\hat{a}_s} \frac{d\hat{a}_s}{dt} \simeq -i\mathcal{E}_s(t) - \langle \hat{\varphi}_s | \nabla_{\mathbb{R}} \hat{\varphi}_s \rangle \cdot \frac{d\vec{\mathcal{R}}}{dt}. \quad (33)$$

Integrating both sides, we get

$$\hat{a}_s(t) = \exp\left[-\frac{i}{\hbar} \int_{t_0}^t \mathcal{E}_s(t') dt'\right] \exp[i\gamma_s] \hat{a}_s(0), \quad (34)$$

the first factor is the complex dynamical phase, whereas the second one is the complex Berry phase given by

$$\gamma_s = i \int_{\mathbf{C}} \langle \hat{\varphi}_s | \nabla_{\mathbb{R}} \hat{\varphi}_s \rangle \cdot d\vec{\mathcal{R}}. \quad (35)$$

Direct evaluation of $\nabla_{\mathbb{R}} |\hat{\varphi}_s\rangle$ requires a locally single valued basis for $|\hat{\varphi}_s\rangle$ and can be awkward. Such difficulties are avoided by transforming the path integral into a surface integral with the help of Stokes theorem

$$\gamma_s = i \sum_{m \neq s} \int_{\Sigma} \int_{\partial\Sigma=\mathbf{C}} \langle \nabla_{\mathbb{R}} \hat{\varphi}_s | \hat{\varphi}_m \rangle \wedge \langle \hat{\varphi}_m | \nabla_{\mathbb{R}} \hat{\varphi}_s \rangle \cdot d\vec{\Sigma}, \quad (36)$$

where Σ is any surface in parameter space whose boundary is the curve \mathbf{C} , and \wedge means wedge product.

This expression may be written in a more convenient form by means of the identity

$$\langle \hat{\varphi}_s | \nabla_{\mathbb{R}} \hat{\varphi}_m \rangle = \frac{1}{\mathcal{E}_m - \mathcal{E}_s} \langle \hat{\varphi}_s | \nabla_{\mathbb{R}} H_1 | \varphi_m \rangle, \quad (37)$$

then,

$$\gamma_s = i \sum_{m \neq s} \int_{\Sigma} \int_{\partial\Sigma=\mathbf{C}} \frac{\langle \hat{\varphi}_s | \nabla_{\mathbb{R}} H_1 | \hat{\varphi}_m \rangle \wedge \langle \hat{\varphi}_m | \nabla_{\mathbb{R}} H_1 | \hat{\varphi}_s \rangle \cdot d\vec{\Sigma}}{(\mathcal{E}_s - \mathcal{E}_m)^2}, \quad (38)$$

provided the surface Σ does not cross any point in D where the denominator vanishes. Since the dependence on $|\nabla_{\mathbb{R}} \varphi_s\rangle$ has been eliminated in (38), phase relations between eigenstates with different parameters are no longer important, any complete set of instantaneous eigenfunctions of the time dependent Hamiltonian H may be used to evaluate the integral in (38).

Explicit expressions for the Berry phase in terms of our parametrization of the interaction Hamiltonian may easily be obtained. Since the unperturbed Hamiltonian and its bound and resonant states are independent of time, the time dependence of the bound and resonant instantaneous energy eigenstates of

the perturbed system is entirely contained in the matrix \mathbf{K} , which is a function of t through the time dependence of the external parameters. Therefore, from eqs.(23), (24) and (25) we get

$$\gamma_s = i \int_{\mathbf{c}} \left[\mathbf{K}^{-1} (\nabla_{\mathfrak{R}} \mathbf{K}) \right]_{ss} \cdot d\vec{\mathfrak{R}}. \quad (39)$$

The columns in $\nabla_{\mathfrak{R}} \mathbf{K}$ are the gradients of the instantaneous eigenvectors of $\mathbf{H}(t)$. Therefore, γ_s may also be written as

$$\gamma_s = i \int_{\mathbf{c}} \langle \phi_s | \nabla_{\mathfrak{R}} \phi_s \rangle \cdot d\vec{\mathfrak{R}}. \quad (40)$$

Furthermore, from (36) we may derive a sum rule for the geometric phases of the interfering resonant states. Writing the integrand in the right hand side of (36) in terms of \mathbf{K} and $\nabla_{\mathfrak{R}} \mathbf{K}$, and taking the sum over s , we get

$$\sum_s \gamma_s = i \int_{\Sigma} \int_{\partial \Sigma = c} \text{tr} \left[(\nabla_{\mathfrak{R}} \mathbf{K}^{-1}) \wedge (\nabla_{\mathfrak{R}} \mathbf{K}) \right] \cdot d\Sigma \quad (41)$$

but

$$-\frac{1}{2\pi} \text{tr} \left[(\nabla_{\mathfrak{R}} \mathbf{K}^{-1}) \wedge (\nabla_{\mathfrak{R}} \mathbf{K}) \right] = C_1(N), \quad (42)$$

is the first Chern class of a complex vector bundle defined by the matrix \mathbf{H} over the parameter space M . Its integral is the first Chern number[25]

$$-\frac{1}{2\pi} \int_{\Sigma} \int_{\partial \Sigma = c} \text{tr} \left[(\nabla_{\mathfrak{R}} \mathbf{K}^{-1}) \wedge (\nabla_{\mathfrak{R}} \mathbf{K}) \right] \cdot d\vec{\Sigma} = c_1. \quad (43)$$

Hence,

$$\sum_s \gamma_s = i \oint \text{tr} \left[\mathbf{K}^{-1} (\nabla_{\mathfrak{R}} \mathbf{K}) \right] \cdot d\vec{\mathfrak{R}} = -2\pi c_1, \quad (44)$$

is a topological invariant.

4 Berry phase factors of resonant states and holonomy in a complex line bundle

4.1 Resonant states as elements of a rigged Hilbert space

Since 1983, B. Simon[15] pointed out that for Hermitian closed quantum systems, the adiabatic evolution can be interpreted as a parallel translation in a Hermitian line bundle and the Berry phase factor is the

holonomy in such a bundle. In this section, it will be shown that this geometric interpretation may be generalized in a very natural way to the Berry phase factor of resonant states of open quantum systems.

The resonant or Gamow functions $\{|\phi_m(\xi_i, \eta_j, r) >\}$ of the unperturbed system are eigenfunctions of the self-adjoint unperturbed Hamiltonian H_0 , which satisfy purely outgoing wave boundary conditions for large values of the separation distance r of the decay fragments. Since the boundary condition is not self-adjoint, the corresponding energy eigenvalues \mathcal{E}_m , are complex, with $Re\mathcal{E}_m > 0$ and $Im\mathcal{E}_m < 0$. In configuration space representation, the Gamow functions, as functions of r , behave as outgoing waves which oscillate between envelopes that increase exponentially. In consequence, Gamow functions are not square integrable and cannot be characterized as elements of a Hilbert space.

Gamow functions are usually associated with the resonance poles of the scattering matrix and the resolvent operator of the time independent Schrödinger equation which lie in the lower half-plane of the unphysical sheet of the Riemann energy surface[1, 12]. In order to give a proper mathematical characterization of Gamow functions as elements of a space, one has to specify a rigged Hilbert space in which the Gamow states $\{|\varphi_m(\xi_i, \eta_j, r) >\}$ are defined as generalized eigenvectors of the Hamiltonian H_0 with generalized complex eigenvalues \mathcal{E}_m .

Following Bohm and Gadella[26], we will associate to the resonant poles of the resolvent operator of the Schrödinger equation of the unperturbed system, a rigged Hilbert space

$$\Phi_+ \subset \mathcal{H} \subset \Phi_+^*, \quad (45)$$

in this expression, Φ_+ is the space of well-behaved functions of the position coordinates (ξ_i, η_j, r) which are Hardy class 2 functions of the complex energy E from above, \mathcal{H} is the Hilbert space of square integrable functions and Φ_+^* is the space of continuous antilinear functionals on Φ_+ . In this way, the Gamow states of the unperturbed system are defined as continuous antilinear functionals on Φ_+ , that is,

$$|\varphi_m(\xi_i, \eta_j, r) > \in \Phi_+^*. \quad (46)$$

The adiabatically evolving Gamow functions $|\hat{\varphi}_s(\xi_i, \eta_j, r; \vec{\mathfrak{R}}(t)) >$ of the complete Hamiltonian H , introduced in section 3, eq.(23), are linear combinations of the Gamow functions $|\varphi_m(\xi_i, \eta_j, r) >$ of H_0 ,

$$|\hat{\varphi}_s(\xi_i, \eta_j, r; [\vec{\mathfrak{R}}(t)]) > = \sum_m |\varphi_m(\xi_i, \eta_j, r) > \mathbf{K}_{ms}[\vec{\mathfrak{R}}(t)], \quad (47)$$

where $\mathbf{K}[\vec{\mathfrak{R}}(t)]$ is the matrix which diagonalizes the complex non-Hermitian matrix $\mathbf{H}[\vec{\mathfrak{R}}(t)]$.

Therefore, the adiabatically evolving Gamow functions are also elements of Φ_+^* ,

$$|\hat{\varphi}_s(\xi_i, \eta_j, r; [\vec{\mathfrak{R}}(t)]) > \in \Phi_+^*. \quad (48)$$

The dual of the Gamow eigenvector $|\hat{\varphi}_s[\vec{\mathfrak{R}}]\rangle$ is the eigenvector $\langle \hat{\varphi}_s[\vec{\mathfrak{R}}]| = \sum_m (\mathbf{K}^{-1})_{sm} \langle \varphi_m(\xi_i, \eta_j)|$ defined in eq.(24), corresponding to the same complex eigenvalue $\mathcal{E}_s[\vec{\mathfrak{R}}]$. Since, by assumption $\mathbf{H}[\vec{\mathfrak{R}}]$ has no repeated eigenvalues for $\vec{\mathfrak{R}}\epsilon\mathbf{C} \subset M$, the adiabatically evolving Gamow eigenvectors and their duals satisfy the orthogonality relation

$$\langle \hat{\varphi}_s[\vec{\mathfrak{R}}]| \hat{\varphi}_{s'}[\vec{\mathfrak{R}}] \rangle = 0, \quad \hat{\mathcal{E}}_s \neq \hat{\mathcal{E}}_{s'} \quad (49)$$

inherited from the Gamow eigenfuctions $|\varphi_m(\xi_i, \eta_j, r)\rangle$ of H_0 , and they may be normalized to one

$$\langle \hat{\varphi}_s[\vec{\mathfrak{R}}]| \hat{\varphi}_s[\vec{\mathfrak{R}}] \rangle = 1 \quad (50)$$

Having characterized the adiabatically evolving Gamow functions as elements of a rigged Hilbert space we may turn to the question of the geometric interpretation of the Berry phase factors of resonant states.

4.2 Adiabatic evolution and parallel translation

Let us suppose that, as time varies, the self-adjoint Hamiltonian $H[\vec{\mathfrak{R}}(t)]$ and its instantaneous energy eigenstates $|\hat{\varphi}_s(\xi_i, \eta_j, r; \vec{\mathfrak{R}}(t))\rangle$ make a cyclic excursion in a closed circuit C in parameter space. We assumed that the time dependence of the Hamiltonian justifies the adiabatic approximation. We will further assume that, if $\vec{\mathfrak{R}}(t)$ is any point on C , the complex matrix $\mathbf{H}[\vec{\mathfrak{R}}(t)]$ has no repeated eigenvalues in an open neighbourhood of $\vec{\mathfrak{R}}\epsilon C$, that is, the Hamiltonian $H(t)$ has no repeated instantaneous complex eigenvalues when $\vec{\mathfrak{R}}\epsilon C$, and that both the generalized eigenvectors $|\hat{\varphi}_s(\xi_i, \eta_j, r; \vec{\mathfrak{R}}(t))\rangle$ and the eigenvalues $\mathcal{E}_s[\vec{\mathfrak{R}}(t)]$ are smooth functions of $\vec{\mathfrak{R}}\epsilon C$. Moreover, we will also assume that the evolution of each state is such that there are no level crossings along C .

To avoid a clumsy notation in the rest of this section we will not write the position coordinates (ξ_i, η_j, r) .

Let us call F_s the complex line bundle defined by the Gamow eigenfunction $|\hat{\varphi}_s[\vec{\mathfrak{R}}(t)]\rangle$ over the parameter space M of the adiabatically evolving system

$$F_s = \left\{ (\vec{\mathfrak{R}}, |\hat{\varphi}_s[\vec{\mathfrak{R}}]\rangle) | H[\vec{\mathfrak{R}}]|\hat{\varphi}_s[\vec{\mathfrak{R}}]\rangle = \mathcal{E}_s[\vec{\mathfrak{R}}]|\hat{\varphi}_s[\vec{\mathfrak{R}}]\rangle, \vec{\mathfrak{R}}\epsilon M \right\} \quad (51)$$

Its fibre is a complex, one-dimensional linear space

$$L_{\vec{\mathfrak{R}}}^s := \left\{ |\hat{\psi}_s[\vec{\mathfrak{R}}]\rangle | |\hat{\psi}_s[\vec{\mathfrak{R}}]\rangle = e^{i\alpha} |\hat{\varphi}_s[\vec{\mathfrak{R}}]\rangle, |\hat{\varphi}_s[\vec{\mathfrak{R}}]\rangle \epsilon \Phi_+^*, \alpha[\vec{\mathfrak{R}}] \epsilon \mathbf{C}^*, \vec{\mathfrak{R}}\epsilon M \right\} \quad (52)$$

where Φ_+^* is the space of antilinear functionals defined over the space Φ_+ of well-behaved functions of Hardy class 2 from above and $\alpha[\vec{\mathfrak{R}}]$ is a complex function of $\vec{\mathfrak{R}}\epsilon M$.

Under the assumptions made above, the quantum number s , labelling the eigenvalue $\hat{\mathcal{E}}_s[\vec{\mathcal{R}}]$ and the eigenstate $|\hat{\varphi}_s[\vec{\mathcal{R}}]\rangle$ of the instantaneous Hamiltonian, is an adiabatic invariant. Hence, a system prepared in a state $|\hat{\psi}_s[\vec{\mathcal{R}}(t)]\rangle$ such that

$$|\hat{\psi}_s[\vec{\mathcal{R}}(t_o)]\rangle = C_s[\vec{\mathcal{R}}(t_o)]|\hat{\varphi}_s[\vec{\mathcal{R}}(t_o)]\rangle \quad (53)$$

will evolve with $H[\vec{\mathcal{R}}(t)]$ and be in a state

$$|\hat{\psi}_s[\vec{\mathcal{R}}(t)]\rangle = C_s[\vec{\mathcal{R}}(t)]|\hat{\varphi}_s[\vec{\mathcal{R}}(t)]\rangle \quad (54)$$

at t .

Now, consider the decomposition of a tangent vector in vertical and horizontal parts

$$\frac{d}{dt}|\hat{\psi}_s(t)\rangle = \left(\frac{d}{dt}|\hat{\psi}_s(t)\rangle\right)_{\parallel} + \left(\frac{d}{dt}|\hat{\psi}_s(t)\rangle\right)_{\perp} \quad (55)$$

The horizontal part, orthogonal to the fibre is

$$\left(\frac{d}{dt}|\hat{\psi}_s(t)\rangle\right)_{\perp} = \sum_{m \neq s} \langle \hat{\varphi}_m[\vec{\mathcal{R}}] | \frac{d}{dt}|\hat{\psi}_s(t)\rangle | \hat{\varphi}_m[\vec{\mathcal{R}}] \rangle \quad (56)$$

and the vertical part, along the fibre is

$$\left(\frac{d}{dt}|\hat{\psi}_s(t)\rangle\right)_{\parallel} = \langle \hat{\varphi}_s[\vec{\mathcal{R}}] | \frac{d}{dt}|\hat{\psi}_s(t)\rangle | \hat{\varphi}_s[\vec{\mathcal{R}}] \rangle \quad (57)$$

If $|\hat{\psi}_s(t)\rangle$ is an evolution state in an adiabatic change,

$$\left(\frac{d}{dt}|\hat{\psi}_s(t)\rangle\right)_{\parallel} = \left(\frac{dC_s[\vec{\mathcal{R}}(t)]}{dt} + \langle \hat{\varphi}_s[\vec{\mathcal{R}}] | \frac{d}{dt}|\hat{\psi}_s(t)\rangle | \hat{\varphi}_s[\vec{\mathcal{R}}] \rangle C_s[\vec{\mathcal{R}}]\right) |\hat{\varphi}_s[\vec{\mathcal{R}}]\rangle \quad (58)$$

The condition for parallel translation along the curve C is

$$\langle \hat{\varphi}_s[\vec{\mathcal{R}}] | \frac{d}{dt}|\hat{\psi}_s[\vec{\mathcal{R}}]\rangle = 0, \quad \vec{\mathcal{R}} \in C \quad (59)$$

which gives a one-form equation

$$dC_s[\vec{\mathcal{R}}] + \langle \hat{\varphi}_s[\vec{\mathcal{R}}] | d\hat{\varphi}_s[\vec{\mathcal{R}}] \rangle C_s[\vec{\mathcal{R}}] = 0 \quad (60)$$

Its solution gives the Berry phase factor of the resonant state

$$\exp[i \int_C \langle \hat{\varphi}_s | d\hat{\varphi}_s \rangle] = \exp[i\gamma_s[\vec{\mathcal{R}}]]. \quad (61)$$

In the case of a cyclic evolution, such that $\vec{\mathcal{R}}(0) = \vec{\mathcal{R}}(T)$ and C is a closed curve, the complex phase γ_s may be expressed as

$$\gamma_s(C) = i \oint_C \langle \hat{\varphi}_s | d\hat{\varphi}_s \rangle. \quad (62)$$

Now, it will be shown that the condition for the adiabatic evolution of a resonant state is equivalent to the condition for parallel translation along C .

The condition for the adiabatic time evolution of a resonant state, equation (33), may be written as

$$e^{-\frac{i}{\hbar} \int_0^t \hat{\mathcal{E}}_s(t') dt'} \left\{ \frac{d}{dt} \left(\hat{a}_s(t) e^{\frac{i}{\hbar} \int_0^t \hat{\mathcal{E}}_s(t') dt'} \right) + \langle \hat{\varphi}_s | \frac{d}{dt} \hat{\varphi}_s \rangle \hat{a}_s(t) e^{\frac{i}{\hbar} \int_0^t \hat{\mathcal{E}}_s(t') dt'} \right\} = 0. \quad (63)$$

Now, making use of the normalization condition, eq.(25), this expressions may be written as

$$e^{-\frac{i}{\hbar} \int_0^t \hat{\mathcal{E}}_s(t') dt'} \langle \hat{\varphi}_s | \vec{\mathcal{R}}(t) \rangle \left\{ |\hat{\varphi}_s[\vec{\mathcal{R}}(t)]| > \frac{dC_s(t)}{dt} + \frac{|d\varphi_s[\vec{\mathcal{R}}(t)]|}{dt} C_s(t) \right\} = 0, \quad (64)$$

where $C_s(t)$ is given by

$$C_s(t) = e^{\frac{i}{\hbar} \int_0^t \hat{\mathcal{E}}_s(t') dt'} \hat{a}_s(t), \quad (65)$$

multiplying both sides of (64) by the dynamic phase factor, the condition for adiabatic evolution of a resonant state takes the form

$$\langle \hat{\varphi}_s | \frac{d}{dt} \hat{\psi}_s \rangle = 0, \quad \vec{\mathcal{R}} \in C \quad (66)$$

which is the condition for parallel translation of the resonant state $|\hat{\psi}_s[\vec{\mathcal{R}}(t)] \rangle = \hat{C}_s[\vec{\mathcal{R}}(t)] |\hat{\varphi}_s[\vec{\mathcal{R}}(t)] \rangle$ along the curve C .

It follows that, except for the effect of the dynamical phase factor, the condition of adiabatic evolution of a resonant state is equivalent to the condition of parallel translation on the complex line bundle F_s .

The geometric phase factors $\exp[i\gamma_s(c)]$, occurring in the adiabatic evolution, are holonomy group elements of the complex line bundle F_s [25].

5 Accidental degeneracy of resonances.

As is apparent from (38), non-trivial phase factors of the energy eigenvectors or eigenfunctions are related to the occurrence of accidental degeneracies of the corresponding eigenvalues. In the absence of symmetry, degeneracies are called accidental for lack of an obvious reason to explain why two energy eigenvalues \mathcal{E}_s and \mathcal{E}_m of \mathbf{H} should coincide. However, if the matrix \mathbf{H} is embedded in a population of complex non-Hermitian matrices $[\mathbf{H}(X_1, X_2, \dots, X_N)]$ smoothly parametrized by N external parameters (X_1, X_2, \dots, X_N) , degeneracy in the absence of symmetry is a geometric property of the hypersurfaces representing the real or complex eigenvalues of \mathbf{H} in a $(N+2)$ -dimensional Euclidean space with Cartesian coordinates $(X_1, X_2, \dots, X_N, \text{Re}\mathcal{E}, \text{Im}\mathcal{E})$.

The energy denominators in (38) show that when the circuit C lies close to a subdomain $D' \subset D$, in parameter space, where the matrix \mathbf{H} has an m -fold repeated eigenvalue, and the state $|\hat{\varphi}_s\rangle$ is involved in this degeneracy, the Berry phase $\gamma_s(c)$ is determined by the geometry of the energy hypersurfaces close to the crossing of eigenvalues and the other $(m-1)$ states involved in the degeneracy.

It is in this connection of the Berry phase with the accidental degeneracy of energy eigenvalues that the non-Hermiticity of the matrix \mathbf{H} plays an important role. In contrast with the case of Hermitian matrices, square, complex, non-Hermitian matrices with repeated eigenvalues cannot always be brought to diagonal form by a similarity transformation. However, any n -dimensional, square complex matrix \mathbf{H} may always be brought to a Jordan canonical form \mathbf{E} by means of a similarity transformation.

If \mathbf{H} has ν ($\nu \leq n$) different eigenvalues, $\mathcal{E}_1, \mathcal{E}_2, \dots, \mathcal{E}_\nu$, with multiplicities $\mu_i(\mathcal{E}_i)$, the Jordan canonical form \mathbf{E} is the direct sum of ν square Jordan blocks \mathbf{E}_i . Each Jordan block \mathbf{E}_i is the sum of a diagonal matrix $\mathcal{E}_i \mathbf{I}_{\mu_i \times \mu_i}$, and a nilpotent matrix N_{μ_i} . Corresponding to each Jordan block, there is a cycle of length μ_i of generalized eigenvectors. When the length μ_i of the cycle is ≥ 2 , the codimension of the accidental degeneracy, the geometry of the energy hypersurfaces at the crossing and the properties of the generalized eigenvectors involved in the degeneracy of resonant states differ substantially from those of bound states([13]). Rather than trying to develop a theory of the most general case, in the following we will examine the simplest possible case, namely the accidental degeneracy of two resonances and the topology of the energy surfaces close to a crossing of two resonances in parameter space.

6 Degeneracy of two resonances

Let us consider a system with two resonant states strongly mixed by a Hermitian interaction, all other bound or resonant eigenstates being non-degenerate. We may suppose that we already know the correct eigenvectors of \mathbf{H} for all the real and complex eigenenergies \mathcal{E}_s , except for the two the crossing of which we want to investigate. Using for this two states two vectors which are not eigenvectors but which are orthogonal to each other and to all other eigenvectors, we obtain a complete basis to represent \mathbf{H} . In this basis, \mathbf{H} will be diagonal except for the elements \mathbf{H}_{12} and \mathbf{H}_{21} . The diagonal elements \mathbf{H}_{11} and \mathbf{H}_{22} will, in general, be non-vanishing and different from each other. There is no loss of generality in this supposition, since any complex matrix \mathbf{H} may be brought to a Jordan canonical form by means of a similarity transformation. When the eigenvalues are equal, $\mathbf{H}_{2 \times 2}$ is either diagonal or equivalent to a Jordan block of rank two. Hence, we need consider only the conditions for degeneracy of the submatrix $\mathbf{H}_{2 \times 2}$.

The matrix $\mathbf{H}_{2 \times 2}$ may be written in terms of the Pauli matrix valued vector $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ and the 2×2 unit matrix as

$$\mathbf{H}_{2 \times 2} = \mathcal{E} \mathbf{1} + \left(\vec{R} - i \frac{1}{2} \vec{\Gamma} \right) \cdot \vec{\sigma}, \quad (67)$$

where \vec{R} and $\vec{\Gamma}$ are real vectors with cartesian components (X_1, X_2, X_3) and $(\Gamma_1, \Gamma_2, \Gamma_3)$. When the forces acting on the system are time reversal invariant, X_2 and Γ_2 vanish.

In the absence of more specific information about the external parameters X , we will parametrize $\mathbf{H}_{2 \times 2}$ in terms of \vec{R} and $\vec{\Gamma}$. Then,

$$\vec{\Re} = \vec{R} - i \frac{1}{2} \vec{\Gamma}. \quad (68)$$

From (67), the eigenvalues of $\mathbf{H}_{2 \times 2}$ are given by

$$\mathbf{E}_{1,2} = \mathcal{E} \mp \epsilon. \quad (69)$$

where

$$\epsilon = \mp \sqrt{\left(\vec{R} - i \frac{1}{2} \vec{\Gamma} \right)^2}. \quad (70)$$

Then, \mathbf{E}_1 and \mathbf{E}_2 coincide when ϵ vanishes. Since, real and imaginary parts of ϵ should vanish, the condition for accidental degeneracy of the two interfering resonances may be written as

$$R_d^2 - \frac{1}{4} \Gamma_d^2 = 0, \quad (71)$$

and

$$\vec{R}_d \cdot \vec{\Gamma}_d = 0. \quad (72)$$

These equations admit two kinds of solutions corresponding to $\mathbf{H}_{2 \times 2}$ being or not being diagonal at the degeneracy:

i) When both \vec{R}_d and $\vec{\Gamma}_d$ vanish, eqs. (71) and (72) define a point in parameter space, \mathbf{H} is diagonal at the degeneracy and the submatrix $\mathbf{H}_{2 \times 2}$ has two cycles of eigenvectors of length one each. The vanishing of Γ_d^2 implies that $Im\mathcal{E}$ also vanishes[13], therefore the two complex eigenvalues of \mathbf{H} which become degenerate fuse into one real positive energy eigenvalue embedded in the continuum. Since in this case all the Cartesian components of \vec{R}_d and $\vec{\Gamma}_d$ should vanish, the minimum number of linearly independent, real, external parameters that should be varied to produce a degeneracy (codimension) of two resonances to form a bound state embedded in the continuum is four or six depending on the quantum system being or not being time reversal invariant.

ii) In the second case, when the degeneracy conditions (71) and (72) are satisfied for non-vanishing \vec{R}_d and $\vec{\Gamma}_d$, these equations define a circle in parameter space. In this case $\mathbf{H}_{2 \times 2}$ is not diagonal at the

degeneracy, it is equivalent to a Jordan block of rank two and has one cycle of generalized eigenvectors of length two. In this case, the two complex eigenvalues become one two-fold repeated eigenvalue \mathcal{E} . Since, the two linearly independent conditions (71) and (72) should be satisfied for non-vanishing values of \vec{R}_d and $\vec{\Gamma}_d$, at least two real, linearly independent parameters should be varied to produce a rank two degeneracy of resonances. Hence, the codimension of a degeneracy of resonances of second rank is two, independently of the time reversal invariance character of the interactions.

6.1 Computation of the geometric phase.

Let us consider now the computation of the Berry phase in the simplest situation when the degeneracy involves only two resonant states. The matrix \mathcal{H} that mixes the two interfering resonances off degeneracy is

$$\mathcal{H} = \begin{pmatrix} Z - i\frac{1}{2}\Gamma & X - iY \\ X + iY & -Z + i\frac{1}{2}\Gamma \end{pmatrix}. \quad (73)$$

This matrix has two right and two left eigenvectors and may be diagonalized by a similarity transformation

$$K^{-1}\mathcal{H}K = \begin{pmatrix} -\epsilon & 0 \\ 0 & \epsilon \end{pmatrix}, \quad (74)$$

where

$$K = \frac{1}{\sqrt{2\epsilon}} \begin{pmatrix} \sqrt{\epsilon + \eta} & \sqrt{\epsilon - \eta} \\ \sqrt{\epsilon - \eta} \frac{\xi^*}{|\xi|} & \sqrt{\epsilon + \eta} \frac{\xi^*}{|\xi|} \end{pmatrix}, \quad (75)$$

ξ and η are short hand for $X - iY$ and $Z - i\frac{1}{2}\Gamma$ respectively. The matrices \mathbf{K}^{-1} and $\nabla_R \mathbf{K}$ are readily obtained from (70) and (75). If we assume that the interfering resonances are mixed by a Hermitian interaction, $\vec{\Gamma}$ will be kept fixed. Then a straightforward calculation gives

$$\gamma_1 = -\frac{1}{2} \int_{\mathbf{c}} \frac{1}{\Gamma \epsilon (\epsilon + \eta)} (\vec{\Gamma} \times \vec{R}) \cdot d\vec{R}, \quad (76)$$

and

$$\gamma_2 = -\frac{1}{2} \int_{\mathbf{c}} \frac{1}{\Gamma \epsilon (\epsilon - \eta)} (\vec{\Gamma} \times \vec{R}) \cdot d\vec{R}. \quad (77)$$

These expressions are very similar to the well known results obtained for the geometric phase of bound states[2]. An obvious difference is that the geometric phase of resonant states is complex since ϵ and η are complex functions of the parameters \vec{R} and $\vec{\Gamma}$. There is another important but less apparent difference: In the case of an accidental degeneracy of resonances ($\Gamma \neq 0$), the denominator in the right hand side of (76)

and (77) vanishes on the continuous line of singularities defined by eqs.(71) and (72), which will be called the diabolical circle, and not at one isolated point as is the case for bound states. It follows that two kinds of non-trivial, topologically inequivalent closed paths are possible. First, those paths which surround the diabolical circle but are not linked to it. Second, the closed paths which are linked to the diabolical circle. Paths of the first kind are clearly analogous to the non-trivial paths that go around the diabolical point of bound state degeneracies while paths of the second kind have no analogue in accidental degeneracies of bound states.

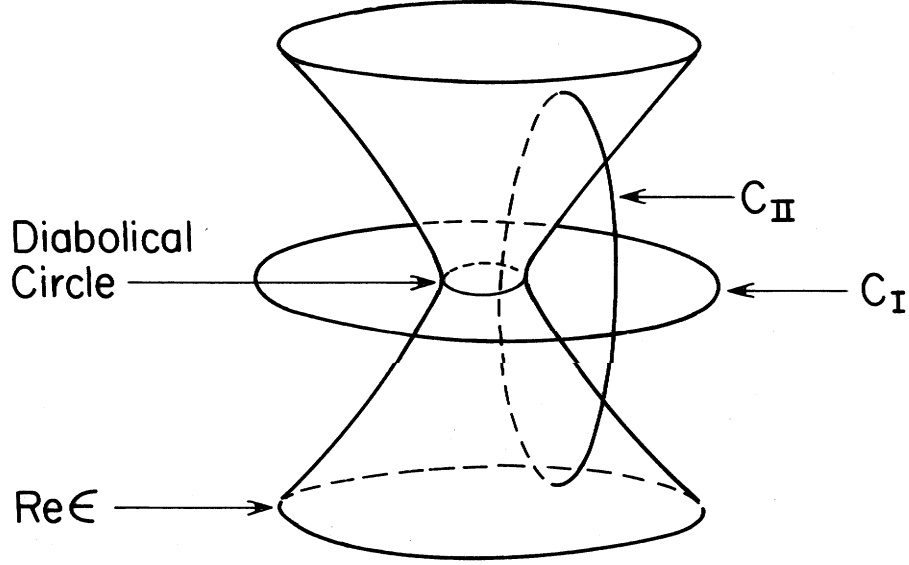


Figure 1: In the evaluation of the Berry phase of two interfering resonant states there are two kinds of non-trivial, topologically inequivalent closed paths in parameter space. First, those, like $C^{(I)}$, which go around the diabolical circle but are not linked to it. Second, those, like $C^{(II)}$, which turn around the diabolical circle and are linked to it.

For paths of the first kind it is always possible to find a surface Σ which spans the closed path \mathbf{C} and does not cross the diabolical circle. Then, Stokes theorem applied to (76) and (77) gives

$$\gamma_s = \frac{(-1)^s}{2} \int_{\Sigma_s} \int_{\partial\Sigma_s=\mathbf{C}} \frac{(\vec{R} - i\frac{1}{2}\vec{\Gamma}) \cdot d\vec{\Sigma}}{\left[(\vec{R} - i\frac{1}{2}\vec{\Gamma})^2\right]^{\frac{3}{2}}}, \quad (78)$$

where $s = 1, 2$. Since γ_2 changes into γ_1 when Σ_1 and Σ_2 are exchanged and the sign of $d\vec{\Sigma}$ is changed, the normals for Σ_2 and Σ_1 should be oppositely oriented. If we say that $\vec{\Gamma}$ points upwards, then Σ_1 is above and Σ_2 is below \mathbf{C} .

This is the same result as would have been obtained from the general expression (38) and our parametriza-

cion of the perturbation term in the Hamiltonian; no summation over intermediate states occurs in (78) since in the simple case of only two interfering resonant states, the summation in (38) has only one term.

Adding γ_1 and γ_2 , we get

$$\gamma_1 + \gamma_2 = -\frac{1}{2} \int_{\Sigma} \frac{(\vec{R} - i\frac{1}{2}\vec{\Gamma}) \cdot d\vec{\Sigma}}{\left[(\vec{R} - i\frac{1}{2}\vec{\Gamma})^2\right]^{\frac{3}{2}}}, \quad (79)$$

where Σ is a sphere with the diabolical circle completely contained in its interior. The integral is easily computed when $R > \frac{1}{2}\Gamma$, the result is

$$-\frac{1}{2\pi}(\gamma_1 + \gamma_2) = 1, \quad (80)$$

in agreement with our identification of the integral in (44) as the first Chern number of the complex line bundle defined by the eigenvector of the non-Hermitian matrix $\mathbf{H}_{2 \times 2}$.

It is now easy to show that the resonance degeneracy produces a continuous distribution of singularities on the diabolical circle. The surface integral in (79) may be written as a volume integral by means of Gauss theorem. Then,

$$\gamma_1 + \gamma_2 = -\frac{1}{2} \int \int \int_V \left(\nabla_R \cdot \frac{(\vec{R} - i\frac{1}{2}\vec{\Gamma})}{\left[(\vec{R} - i\frac{1}{2}\vec{\Gamma})^2\right]^{\frac{3}{2}}} \right) dV, \quad (81)$$

where V is the volume inside Σ and bounded by it. The term in round brackets under the integration sign vanishes when $(\vec{R} - i\frac{1}{2}\vec{\Gamma})^2 \neq 0$. Therefore, the non-vanishing value of $\gamma_1 + \gamma_2$ implies the occurrence of δ -function singularities of the integrand on those points where $(\vec{R} - i\frac{1}{2}\vec{\Gamma})^2$ vanishes.

Hence,

$$\nabla_R \cdot \left[\frac{\vec{R} - i\frac{1}{2}\vec{\Gamma}}{\left[(\vec{R} - i\frac{1}{2}\vec{\Gamma})^2\right]^{\frac{3}{2}}} \right] = -\frac{\delta(R - \frac{1}{2}\Gamma)}{R^2} \delta(\cos \theta), \quad (82)$$

the factor R^{-2} multiplying the delta function is needed to reproduce the value 2π of $\gamma_1 + \gamma_2$.

Let us turn to the case of closed paths of the second kind, that is, those paths which are linked to the diabolical circle. In this case there is no surface Σ which spans the closed path c^{II} without crossing the diabolical circle. Therefore, it is not possible to use Stokes theorem to convert the path integral into a surface integral. However, we may still compute the geometric phase from the path integral. To this end, we change from Cartesian coordinates (X, Y, Z) with OZ parallel to $\vec{\Gamma}$, to spherical coordinates in parameter space. Then, eqs. (76) and (77) take the form

$$\gamma_{1,2} = -\frac{1}{2} \int_c d\varphi \mp \frac{1}{2} \int_c \frac{\left(R \cos \theta - i\frac{1}{2}\Gamma\right) d\varphi}{\sqrt{R^2 - \frac{1}{4}\Gamma^2 - i\Gamma R \cos \theta}}, \quad (83)$$

the path c is specified when R and θ are given as functions of φ .

From (83), it follows that, for closed paths which are linked to the diabolical circle,

$$\gamma_1 + \gamma_2 = - \int_{c^{(II)}} d\varphi = 0, \quad c^{(II)} \text{ of second kind} \quad (84)$$

since, in this case, the angle φ starts out at some value φ_0 and, as the system traces the path c^{II} , it oscillates between a minimum and a maximum values and finally ends at the same initial value φ_0 . There is no analogue to this case in the geometric phase of bound states.

7 Results and conclusions

The purpose of the foregoing has been to discuss the geometric phase acquired by the resonant states when they are adiabatically transported in parameter space around a degeneracy of resonances .

As in the case of bound states, the condition of adiabatic evolution of resonant states may be given a geometric interpretation as parallel translation in a complex line bundle F_s . The geometric phase factors acquired by the resonant states when adiabatically transported in a closed circuit in parameters space are holonomy group elements of the complex line bundle F_s .

In the case of two resonant states mixed by a Hermitian interaction we find two kinds of accidental degeneracies which may be characterized by the number and length of the cycles of instantaneous energy eigenfunctions at the degeneracy. In the first case there are two linearly independent eigenfunctions belonging to the same real positive repeated energy eigenvalue, that is, two cycles of lenght one. In the second case there is only one resonant eigenstate and one generalized resonant eigenstate belonging to the same degenerate (repeated) complex energy eigenvalue, *i.e.* one cycle of lenght two. At degeneracy, the Hamiltonian matrix has one Jordan block of second rank.

In the generic case of a non-time reversal invariant system, when the degeneracy is of the second rank, the topology of the energy surfaces is different from that at a crossing of bound states. The energy surfaces of the two resonant states that become degenerate touch each other at all points in a circle. Close to the crossing, the energy hypersurface has two pieces lying in orthogonal subspaces in parameter space. The surface representing the real part of the energy has the shape of a hyperbolic cone of circular cross section, or an open sandglass, with its waist at the diabolical circle. The surface of the imaginary part of the energy is a sphere with the equator at the diabolical circle. The two surfaces touch each other at all points on the diabolical circle[13].

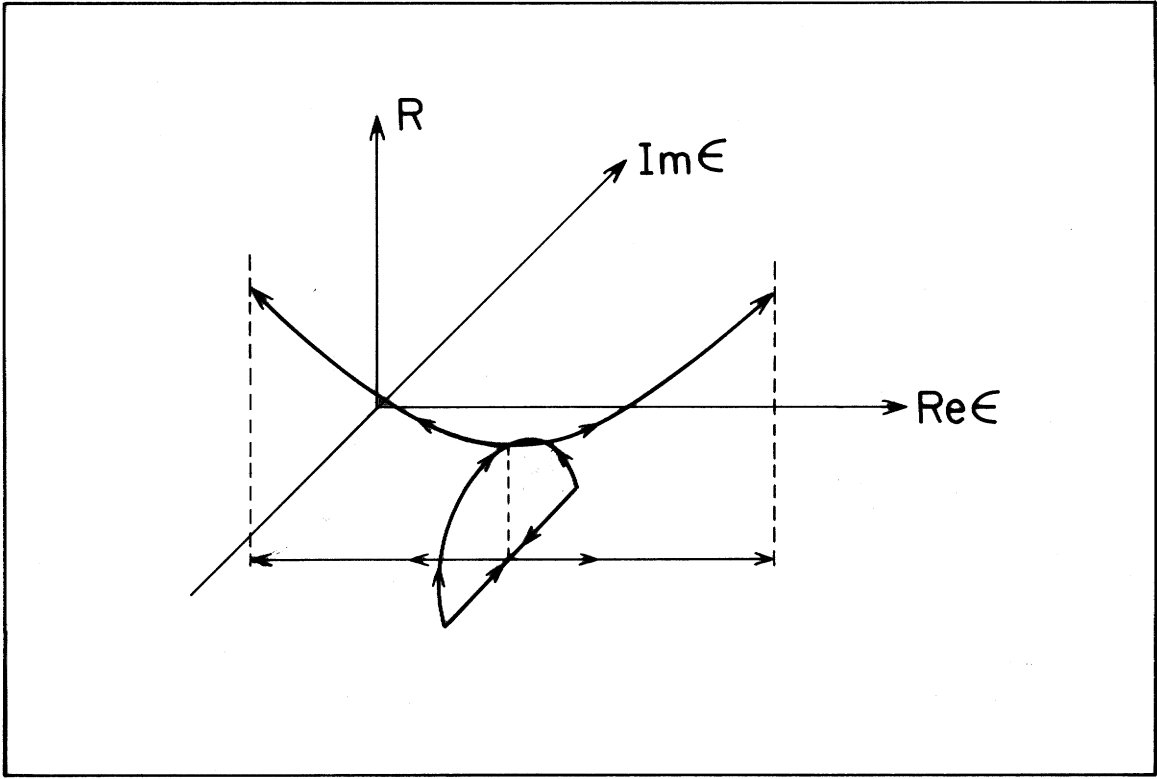


Figure 2: Two interfering resonances which initially have equal level energies but different half widths are mixed by the Hermitian interaction $\vec{R} \cdot \vec{\sigma}$. As R increases from 0 to $\frac{1}{2}\Gamma$, the points representing \mathcal{E}_1 and \mathcal{E}_2 approach each other along a meridian circle on the sphere representing $Im\epsilon$ in parameter space, until they meet at a point on the equator, which is the diabolical circle. At this point the two resonances become degenerate and the mixing matrix \mathbf{H}_d is equivalent to a Jordan block of rank two. When R becomes larger than $\frac{1}{2}\Gamma$ the points representing \mathcal{E}_1 and \mathcal{E}_2 move away from each other on the hyperbolic cone representing $Re\epsilon$.

In the case of two interfering resonant states, the geometric phase acquired by the resonant states when transported around the diabolical circle in a closed path which is not linked to it, may be written as the sum of two terms.

$$\gamma_{1,2}^{res}(\mathbf{c}^I) = \gamma_{1,2}^{bound}(\mathbf{c}^I) \pm \Delta\gamma(\mathbf{c}^I). \quad (85)$$

The first term, $\gamma_{1,2}^{bound}(\mathbf{c}^I)$, is the real geometric phase which a negative energy eigenstate would have acquired when transported around a diabolical point in a closed path in the same parameter space. The second term is complex, it gives rise to a change of the phase and a dilation of the resonant state eigenfunction. Its imaginary part may be positive or negative, in consequence, it may produce an amplification or a damping of the wave function which may compensate or reinforce the attenuation due to the imaginary

part of the dynamical phase factor.

When the resonant states are transported in a closed path \mathbf{c}^{II} which does not go around the diabolical circle but is linked to it, the geometric phase they acquire is

$$\gamma_{1,2}^{res}(\mathbf{c}^{II}) = \pm \Delta\gamma(\mathbf{c}^{II}). \quad (86)$$

Since it is not possible to find a continuous surface Σ which spans the closed path \mathbf{c}^{II} without crossing the diabolical circle, we can not make use of the theorem of Stokes to convert the path integral into a surface integral. However, it may readily be computed as a path integral from the expression

$$\Delta\gamma(\mathbf{c}^{II}) = \int_{\mathbf{c}^{II}} \frac{(Z - i\frac{1}{2}\Gamma)(\vec{\Gamma} \times \vec{R}') \cdot d\vec{R}'}{\Gamma \sqrt{(\vec{R} - i\frac{1}{2}\vec{\Gamma})^2 (X^2 + Y^2)}}, \quad (87)$$

which is obtained from (83) and (84). As in the previous case, $\Delta\gamma(\mathbf{c}^{II})$ is complex and produces changes of phase and dilations in the resonant state wave function. This case has no analogue in bound states.

The sum of the geometric phases acquired by two interfering resonant states which are transported around a degeneracy in a closed path of the first kind in parameter space is a topological invariant, namely the first Chern number[25]. Its value is the “magnetic charge” on the diabolical circle. For paths of the second kind the sum of the geometric phases vanishes.

References

- [1] Bohm A, *Quantum Mechanics: Foundations and Applications*, 3rd Edn. New York, Springer-Verlag 1993, Ch. XXI
- [2] Berry M. V. *Proc. Roy. Soc.* **A392**,45, (1984)
- [3] For reviews on Berry’s phase see: Jackiw, R. *Commun. At. Mol. Phys.* **27**, 71, (1988); Vinitiskii S.J., Derbov V.L., Dubovik V.N., Markovski B.L. and Stepanovskii Yu. P. *Sov.Phys. Usp.* **33**, 403, (1990); Moore J.D. *Phys. Rep.* **210** , 1, (1990).
Zwanziger J.W., Rucker S.P. and Chingas, G.C. *Phys. Rev.* **A43**, 3232, (1991)
Alden Mead, G. *Rev. Mod. Phys.*, **64**, 51, (1992)
- [4] For collections of basic papers on geometric phases see the monographs: Wilckzek F. and Shapere A. (Eds) *Geometric Phases in Physics* Singapore: World Scientific, 1989.
Markovsky B. and Vinitsky V.I. (Eds) *Topological Phases in Quantum Theory*. Singapore: World Scientific 1989.

- [5] Dattoli G., Mignani R. and Torre A. *J. Phys. A: Math Gen.* **23**, 5795, (1990)
- [6] Miniatura Ch., Sire C., Baudon J. and Bellissard J. *Europhys. Lett.* **13**, 199, (1990).
- [7] Nenciu, G. and Rasche G. *J. Phys. A: Math. Gen.* **25**, 5741, (1992).
- [8] Kvitsinsky, A. and Putterman, S. *J. Math. Phys.* **32**, 1403, (1991).
- [9] Sun, C.P. *Phys. Scr.* **48**, 393, (1993).
- [10] Hernández E., Jáuregui A. and Mondragón A. *Rev. Mex. Fis.* **38** (S2), 128, (1992).
- [11] Mondragón A. and Hernández E. *J. Phys. A: Math. Gen.* **29**, 2567, (1996).
- [12] Mondragón A., Hernández E. and Velázquez-Arcos J.M. *Ann. Phys. (Leipzig)* **48**, 503, (1991).
- [13] Mondragón A. and Hernández E. *J. Phys. A: Math. Gen.* **26**, 5595, (1993).
- [14] Hernández E. and Mondragón A. *Phys. Lett.* **326B**, 1, (1994).
- [15] Simon B. *Phys. Rev. Lett.* **51**, 2167 (1983).
- [16] Satchler, G.R. *Direct Nuclear Reactions*. London. Oxford University Press 1983 Ch. 3 and references therein.
- [17] Tang Y.C. *Microscopic description of nuclear cluster theory in: Topics in Nuclear Physics II* Lectures Notes in Physics 145 Eds. T.T.S. Kuo and S.S.M. Wong New York Springer 1981.
- [18] Romo W.J. *Nucl. Phys.* **A116**, 618, (1968).
- [19] Hardy G.H, *Divergent Series*. Oxford, Clarendon Press 1949.
- [20] Zel'dovich Ya. B. *JETP (Sov. Phys.)* **12**, 542, (1961).
- [21] Berggren T. *Nucl. Phys.* **A109**, 265 (1968).
- [22] Gyarmati B. and Vertse T. *Nucl. Phys.* **A160**, 523, (1971).
- [23] Gyarmati, B., Kruppa A.T. and Papp Z. *Phys. Rev.* **C31**, 2317, (1985).
- [24] Hernández E. and Mondragón A. *Phys. Rev.* **C29**, 722, (1984).
- [25] Nakahara N. *Geometry, Topology and Physics* Bristol: Adam Hilger, 1990.
- [26] Bohm, A. and Gadella M. *Dirac Kets, Gamow Vectors and Gel'fand Triplets* in: Lecture Notes in Physics **348**. Berlin Springer-Verlag 1989.